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CAREER: Ferroelectric Multilayers, Superlattices, and Compositionally Graded Films

DMR-0132918; PI: S. Pamir Alpay/University of Connecticut

People

During the past 6 months, 2 graduate students, 3 undergraduate students and 1 summer intern were supported by the NSF grant. Mr. Zhigang Ban is a Materials Engineering Ph. D. student from the People's Republic of China and works on the theoretical modeling of ferroelectric multilayers and graded films. Mr. Burc Misirlioglu is a Ph. D. student in the Materials Engineering Department from Turkey. He is mainly involved in the synthesis of the films via pulsed laser deposition. Mr. Dean Halter, Mr. Scott Virkler, and Mr. Michael White are Mechanical Engineering seniors who double major in Materials Engineering. Ms. Anna Chabaeva has recently joined our group as a summer intern. She is conducting literature search and analysis of crystallographic, structural and electrical properties of KNO/KTO ferroelectric superlattices.

Outreach

The technologically important aspects of this program work is related to the current and potential applications of thin films in the microelectronics and automotive sectors. One of the more ambitious features of the program is the development of a state-of-the-art "popular science" web site on thin film technology, their applications and future prospects that will appeal to a general audience, particularly high school teachers, juniors and seniors.

Such a web site was recently developed and uploaded to a UConn server thanks to the efforts of Mr. Halter, Mr. White, and Mr. Virkler who are Mechanical Engineering seniors double-majoring in Materials Engineering. During the past six months, they have worked not only on the design of the web pages but on the content as well. The address of the web site is: http://www.ims.uconn.edu/~alpay/thinfilms/index.html. The main page of the web site is shown in the figure above. Although far from complete, the web pages already contain extensive information on thin film deposition techniques, SEM, TEM, and AFM images of thin films, schematics of the deposition methods, and animations.

The web site is also submitted to popular search engines such as yahoo.com and msn.com. Collaboration with the Materials Research Society (MRS) is sought in order to attract a more technical audience and prospective graduate students.

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Amount: \$517,164

Duration: 12/15/01 to 11/30/06

This CAREER project focuses on the engineering of artificially layered ferroelectric superlattices and compositionally graded ferroelectric films (Figure 1) with enhanced properties through spatial variations in internal stresses, film composition, and microstructure. Making use of the unique intrinsic characteristics of ferroelectric materials and introducing compositional and internal stress gradients, exceptional and unusual electrical and electromechanical properties can be obtained which are not possible for bulk ferroelectrics and ferroelectric thin films.

The proposed work is a combined experimental and theoretical effort. The interactions between individual layers will be modeled and physical properties of ferroelectric multilayers and compositionally graded films will be determined. Ferroelectric and/or paraelectric layers with systematic variations in composition, thickness, and misfit with respect to the underlying substrate will be deposited by pulsed lased deposition. We have focused on the deposition of the prototypical BaTiO₃/SrTiO₃ system. Based on the information gathered, multilayers of other perovskite systems such as PbTiO₃/CaTiO₃, PbTiO₃/SrTiO₃, and KNbO₃/KTaO₃, will be grown. Ferroelectric stacks and compositionally graded films will be characterized crystallographically and microstructurally via x-ray diffraction and transmission electron microscopy. Local compositional distribution of elements will be determined by energy-dispersive x-ray spectroscopy (EDXS) using an electron energy filter. The physical properties such as the polarization hysteresis, dielectric, piezoelectric, and pyroelectric properties will be measured.

Based on theoretical and experimental results, the design and production of fundamentally new devices and circuit structures will become possible. These devices will have applications as chip capacitors, sensors/actuators for MEMS, and infrared pyroelectric sensors, exploiting not only the enhanced dielectric, piezoelectric, and pyroelectric properties of ferroelectric multilayers and compositionally graded films but also the "built-in" electrical field shown in Figure 2 [D. Bao, N. Mizutani, L. Zhang, and X. Yao, *J. Appl. Phys.*, **89**, 801 (2000)]. One of the possibilities for compositionally graded ferroelectric films are trans-capacitive, or "transpacitor," ferroelectric devices, which store charge and generate voltage.